III International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2013
M. Bischoff, E. Oñate, D.R.J. Owen, E. Ramm & P. Wriggers (Eds)

MODELLING OF SOLID BODIES IN DISSIPATIVE PARTICLE DYNAMICS

N. MAI-DUY[1,2], N. PHAN-THIEN[2], B.C. KHOO[2] AND T. TRAN-CONG[1]

[1] Computational Engineering and Science Research Centre,
Faculty of Engineering and Surveying,
University of Southern Queensland, QLD 4350, Australia
nam.mai-duy@usq.edu.au, thanh.tran-cong@usq.edu.au

[2] Department of Mechanical Engineering,
Faculty of Engineering,
National University of Singapore, Singapore
Email: nhan@nus.edu.sg, mpekbc@nus.edu.sg

Key words: dissipative particle dynamics, particulate suspensions, spring model, soft potential, thermodynamic temperature

Abstract. This paper is concerned with the use of oscillating particles instead of the usual frozen particles to model a suspended particle (solid body) in a Dissipative Particle Dynamics (DPD) particle-based simulation method. A suspended particle is represented by a set of basic DPD particles connected to reference sites by linear springs. The reference sites are moved as a whole with the imposed displacement that is calculated using data from the previous time step, while the velocities of their associated DPD particles are found by solving the DPD equations at the current time step. In this way, a specified Boltzmann temperature can also be maintained in the region occupied by the suspended particles and this parameter can be utilised to control the size of suspended particles. Several numerical results in two dimensions are presented to demonstrate attractiveness of the proposed model.

1 INTRODUCTION

Dissipative Particle Dynamics (DPD), which was proposed by Hoogerbrugge and Koelman in 1992 [1], is a mesoscopic simulation technique for complex fluid systems. Its formulation is derived from the view that each DPD particle represents a group of molecules. DPD particles interact through a soft potential and thus the simulation can be carried out on length and time scales far beyond those of Molecular Dynamics (MD). Hydrodynamic interactions are accounted by employing velocity-dependent dissipative forces. It should be pointed out that ensemble-average quantities formed from the DPD particle states (configurations and velocities) satisfy conservation of mass and momentum [2]. One of the most attractive features of DPD is that its ability to model complex fluids in a simple way. A subset of DPD particles can be constrained to form a solid object, a droplet, a polymer chain, etc.

This study is concerned with the simulation of particulate suspensions. We propose a simple model, where a suspended particle is represented by using a small set of basic DPD particles that fully interact with each other and with the rest of DPD particles. For example, a hard disk (2D circular cylinder) is assumed to be made up of 4 basic DPD particles only. The constituent particles of a colloidal particle are connected to the reference site via linear springs. This allows a specified thermodynamic temperature to be maintained over the entire domain and one can use this parameter to control the effective size of the colloidal particles. For the latter, a larger size of the suspended particle can be achieved at a negligible extra computational cost. Another computational advantage of the proposed model is that the present DPD parameters are the same as those for the single fluid case. It means that (i) the underlying particles all interact through a soft potential (linear forces) and thus make large time steps in the suspension simulation possible; and (ii) all interactions between particles can use the same cutoff radius and therefore allow one to use a simple, single level linked-list algorithm.

The remainder of the paper is organised as follows. Section 2 provides a brief overview of the standard DPD equations. The proposed spring model for suspended particles is described in Section 3 and then verified numerically in Section 4. Section 5 gives some concluding remarks.

2 DISSIPATIVE PARTICLE DYNAMICS

The stochastic differential equations governing the motion of a DPD particle are given by

$$\dot{\mathbf{r}}_i = \mathbf{v}_i, \tag{1}$$

$$m_i \dot{\mathbf{v}}_i = \mathbf{F}_i, \tag{2}$$

where m_i, $\mathbf{r}_i$ and $\mathbf{v}_i$ represent the mass, position and velocity vector of a particle $i = 1, \ldots, N$, respectively, N is the total number of DPD particles, the superposed dot denotes a time derivative, and $\mathbf{F}_i$ is the total force vector exerted on particle i, containing three parts

$$\mathbf{F}_i = \sum_{j=1, j\neq i}^{N} \left(\mathbf{F}_{ij,C} + \mathbf{F}_{ij,D} + \mathbf{F}_{ij,R}\right), \tag{3}$$

in which the sum runs over all other particles except i, within a certain cutoff radius r_c. Outside the cutoff radius (which is the same for $\mathbf{F}_{ij,D}$ and $\mathbf{F}_{ij,R}$ but may be different for $\mathbf{F}_{ij,C}$), these forces are set to zero. The first term on the right is referred to as conservative force (subscript C), the second, dissipative force (subscript D) and the third, random force (subscript R). These forces are pairwise and are usually given in the forms

$$\mathbf{F}_{ij,C} = a_{ij} w_C \mathbf{e}_{ij}, \tag{4}$$

$$\mathbf{F}_{ij,D} = -\gamma w_D \left(\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}\right) \mathbf{e}_{ij}, \tag{5}$$

$$\mathbf{F}_{ij,R} = \sigma w_R \theta_{ij} \mathbf{e}_{ij}, \tag{6}$$

where a_{ij}, γ and σ are constants reflecting the strengths of these forces, w_C, w_D and w_R the distance-dependent weighting functions, $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ a unit vector from particle j to particle i ($\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$), $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ the relative velocity vector, and θ_{ij} a Gaussian white noise ($\theta_{ij} = \theta_{ji}$) with stochastic properties

$$\langle \theta_{ij} \rangle = 0, \tag{7}$$

$$\langle \theta_{ij}(t)\theta_{kl}(t') \rangle = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\delta\left(t - t'\right), \text{with } i \neq k \text{ and } j \neq l. \tag{8}$$

It was shown in [3] that the following

$$w_D(r_{ij}) = \left(w_R(r_{ij})\right)^2, \tag{9}$$

$$k_B T = \frac{\sigma^2}{2\gamma}, \tag{10}$$

lead to a detailed balance of the system (equi-partition principle or fluctuation-dissipation theorem), which relate the strength of the dissipative force to the strength of the random force through the definition of the thermodynamic temperature (constant fluctuation kinetic energies). A popular choice of the weighting functions is

$$w_C(r_{ij}) = 1 - \frac{r_{ij}}{r_c}, \tag{11}$$

$$w_D(r_{ij}) = \left(1 - \frac{r_{ij}}{r_c}\right)^s. \tag{12}$$

where s is a constant ($s = 2$ and $s = 1/2$ are two typical values of s).

There are two relevant time scales in the simulation of particulate suspensions - (i) the time over which Brownian diffusion restores the equilibrium configuration: a^2/D_0 (a is the sphere radius and D_0 the single-sphere diffusion coefficient), and (ii) the time needed to deform the microstructure by shear: $1/\dot{\gamma}$ ($\dot{\gamma}$ the shear rate). The Peclet number is defined as the ratio between the two time scales $Pe = \dot{\gamma}a^2/D_0$. This number measures the relative important of hydrodynamic and Brownian contributions to the flow.

3 PROPOSED MODEL FOR A SUSPENDED PARTICLE

We propose to model a suspended particle by a set of p basic DPD particles (p is small) connected to reference sites by linear springs. For example, a hard disk (2D cylinder of circular shape) is constructed here using 4 basic DPD particles only ($p = 4$) (Figure 1).

Consider the kth suspended particle. The base, which is comprised of reference sites as illustrated in Figure 2, is assumed (i) to move as a whole and (ii) to have a negligible mass. For the former, certain pairs of sites are required to satisfy the condition

$$\xi_{ij}^k(t) \equiv \left(\bar{\mathbf{r}}_i^k(t) - \bar{\mathbf{r}}_j^k(t)\right)^T \left(\bar{\mathbf{r}}_i^k(t) - \bar{\mathbf{r}}_j^k(t)\right) - \left(d_{ij}^k\right)^2 = 0, \tag{13}$$

where d_{ij} is the fixed distance between sites i and j, and the overline is used to differentiate the site from its associated DPD particle.

The location of the mass centre of the kth colloidal particle is computed as

$$\mathbf{R}_c^k = \frac{1}{M_c^k}\left(\sum_{i=1}^{p} m_i \mathbf{r}_i^k + \sum_{i=1}^{p} \overline{m}_i \bar{\mathbf{r}}_i^k\right) \approx \frac{1}{M_c^k}\left(\sum_{i=1}^{p} m_i \mathbf{r}_i^k\right), \quad M_c^k = \sum_{i=1}^{p} m_i + \sum_{i=1}^{p} \overline{m}_i \approx \sum_{i=1}^{p} m_i, \tag{14}$$

where M_c^k is the total mass of the kth colloidal particle.

The force on a constituent particle of the suspended particle is

$$\mathbf{F}_i^k(t) = m_i \dot{\mathbf{v}}_i^k = \sum_{j=1, j\neq i}^{N} \left[\mathbf{F}_{ij,C}^k(t) + \mathbf{F}_{ij,D}^k(t) + \mathbf{F}_{ij,R}^k(t)\right] + \mathbf{F}_{i,S}^k(t), \quad i = (1, 2, \cdots, p), \tag{15}$$

where $\mathbf{F}_{i,S}^k(t) = -H\left[\mathbf{r}_i^k(t) - \bar{\mathbf{r}}_i^k(t)\right]$ is the spring force with H being the stiffness of the spring. In the limit $H \to \infty$, one has $\mathbf{r}_i^k(t) \to \bar{\mathbf{r}}_i^k(t)$. As a result, the centre of mass of the system is also the centre of the reference sites. In the present work, the value of H is chosen quite large.

The force on a reference site of the suspended particle is

$$\overline{\mathbf{F}}_i^k(t) = \overline{m}_i \dot{\overline{\mathbf{v}}}_i^k = \overline{\mathbf{F}}_{i,S}^k(t) + \mathbf{G}_i^k(t), \quad i = (1, 2, \cdots, p), \tag{16}$$

where $\overline{\mathbf{F}}_{i,S}^k$ and $\mathbf{G}_i^k$ are the spring and constraint forces, respectively. The latter is given by

$$\mathbf{G}_i^k(t) = -\sum_{j=1} \lambda_{ij}(t) \nabla_i \xi_{ij}(t), \tag{17}$$

where $\lambda_{ij}(t)$ are the time-dependent Lagrange multipliers and ∇_i is the gradient with respect to the coordinates of the reference site under consideration. Note that $\lambda_{ij}(t) = \lambda_{ji}(t)$, $\xi_{ij}(t) = \xi_{ji}(t)$ and $\nabla_i \xi_{ij}(t) = -\nabla_j \xi_{ij}(t)$.

Using (15) and (16), the net force and torque on the kth colloidal particle are expressed as

$$\mathbf{F}^k = \sum_{i=1}^{p} \mathbf{F}_i^k(t) + \sum_{i=1}^{p} \overline{\mathbf{F}}_i^k(t), \tag{18}$$

$$\mathbf{T}^k = \sum_{i=1}^{p} \left(\mathbf{r}_i^k - \mathbf{R}_c^k\right) \times \mathbf{F}_i^k(t) + \sum_{i=1}^{p} \left(\bar{\mathbf{r}}_i^k - \mathbf{R}_c^k\right) \times \overline{\mathbf{F}}_i^k(t). \tag{19}$$

Since the constraint forces and also the spring forces are pairwise and the two forces in each pair are equal in magnitude and opposite in direction, expressions (18) and (19) reduce to

$$\mathbf{F}^k = \sum_{i=1}^{p} \sum_{j=1, j\neq i}^{N} \left[\mathbf{F}^k_{ij,C}(t) + \mathbf{F}^k_{ij,D}(t) + \mathbf{F}^k_{ij,R}(t)\right], \tag{20}$$

$$\mathbf{T}^k = \sum_{i=1}^{p} \left(\mathbf{r}^k_i - \mathbf{R}^k_c\right) \times \sum_{j=1, j\neq i}^{N} \left[\mathbf{F}^k_{ij,C}(t) + \mathbf{F}^k_{ij,D}(t) + \mathbf{F}^k_{ij,R}(t)\right]. \tag{21}$$

It should be pointed out that the sum of the spring forces on the constituent particles of the colloidal particle are absent in the net force and torque on the colloidal particle.

The velocity of the mass centre and the angular velocity of the kth colloidal particle are derived from

$$M^k_c \frac{d\mathbf{V}^k_c}{dt} = \mathbf{F}^k(t), \tag{22}$$

$$\mathbf{I}^k \frac{d\boldsymbol{\omega}^k}{dt} = \mathbf{T}^k(t) + \boldsymbol{\omega}^k \times (\mathbf{I}^k \boldsymbol{\omega}^k), \tag{23}$$

where $\mathbf{I}^k$ is the moment of inertia tensor.

A set of reference sites is advanced according to

$$\frac{d\bar{\mathbf{r}}_i}{dt} = \mathbf{V}^k_c + \boldsymbol{\omega}^k \times \left(\bar{\mathbf{r}}^k_i - \mathbf{R}^k_c\right), \quad i = (1, 2, \cdots, p), \tag{24}$$

while the corresponding velocities of the constituent particles are to be found from solving equation (15).

In the present model, values used in the DPD interactions between constituent-constituent particles and between constituent-solvent particles are exactly the same as those between solvent-solvent particles. Unlike the frozen-particle models [4], the present constituent particles have an additional oscillatory motion about their associated reference sites. There exist dissipative forces between the constituent particles. A specified constant thermodynamic temperature can be maintained throughout the domain. In contrast to to the single-particle models [5], the present underlying particles all interact through a soft potential (soft repulsive particles), and there is one type of interaction only in the system: the interaction between two basic particles.

4 NUMERICAL EXAMPLES

The model system we consider here comprises an ensemble of disks immersed in a 2D fluid. We now model a suspended hard disc (2D cylinder) using a set of only 4 DPD particles whose associated reference sites are located on a square of the side length 0.25 (DPD units). Parametric values for the DPD forces on these constituent particles are the same as those on the solvent particles. The simulation is carried out on the domain 10×10 with the following DPD parameters: $m_i = 1$, $s = 1/2$, $n = 4$, $a_{ij} = 18.75$, $\sigma = 3$ and $r_c = 1$. After some investigation, a linear spring of the same stiffness $H = 3000$ is used.

Consider the case of one colloidal particle. The variations of spring forces on the particle with respect to the number of time steps are shown in Figure 3. There exist spring forces on its constituent particles. However, the sum of these spring forces is very small as expected (the base containing reference sites is assumed to have a negligible mass). It appears that the spring force on a constituent particle has a zero mean.

We use the radial distribution function to measure the effective size of the particle

$$g(q) = \frac{1}{N/A} \frac{p}{2\pi q \Delta q}, \tag{25}$$

where A is the area of the domain containing N particles and p is the number of particles in a circular shell of width $q \to (q+\Delta q)$ at a distance q from the particle under consideration. We investigate the effect of $k_B T$ on the particle size. Two values of $k_B T$, 0.5 and 1, are considered. Figure 4 shows the variation of $g(q)$, where Δq is chosen as 0.01, for the present DPD fluid and for the single disk embedded in the fluid.

It can be seen that the radius of exclusion zone ($g \approx 0$) for the colloidal particle is increased from 0.4 to 0.5 as $k_B T$ is reduced from 1 to 0.5. A larger size of the colloidal particle is achieved at a negligible extra computational cost. The present model thus allows one to effectively control the effective size of the colloidal particle through the thermodynamic temperature.

Figure 5 shows percentage errors of the average value of kBT versus volume fraction between the present oscillating and frozen particle models. It can be seen that the former is much more accurate than the latter for all values of volume fraction.

Results concerning the relative viscosity of the suspension over a wide range of volume fraction by the present model, the fictitious-domain/finite-element method [6] and several empirical formulas [7, 8] are shown in Figure 6. Results for the case of dilute suspensions [9] are also included. The present results agree well with those by the empirical formulas.

All simulations presented in this study are conducted with $\Delta t = 0.01$ - a relatively large time step.

5 CONCLUDING REMARKS

In this paper, we present a simple DPD model for particulate suspensions, where only standard DPD forces and spring forces are included and a suspended particle is represented by a few oscillating DPD particles. The present model yields a good prediction for the zero-shear-rate relative viscosity over a wide range of the volume fraction.

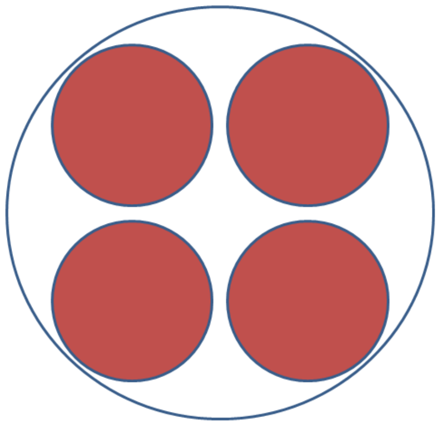

Figure 1: A circular disk is represented using 4 basic DPD particles.

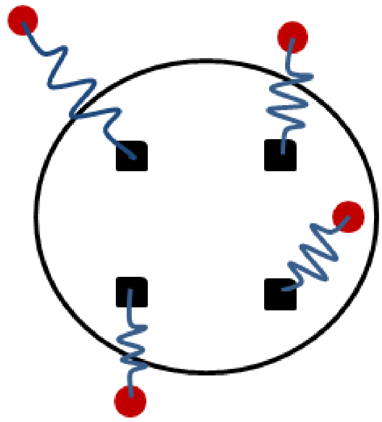

Figure 2: A schematic diagram for the proposed spring model: DPD particles (circles) connected to reference sites (squares) via linear springs. There are rigid constraints between the reference sites.

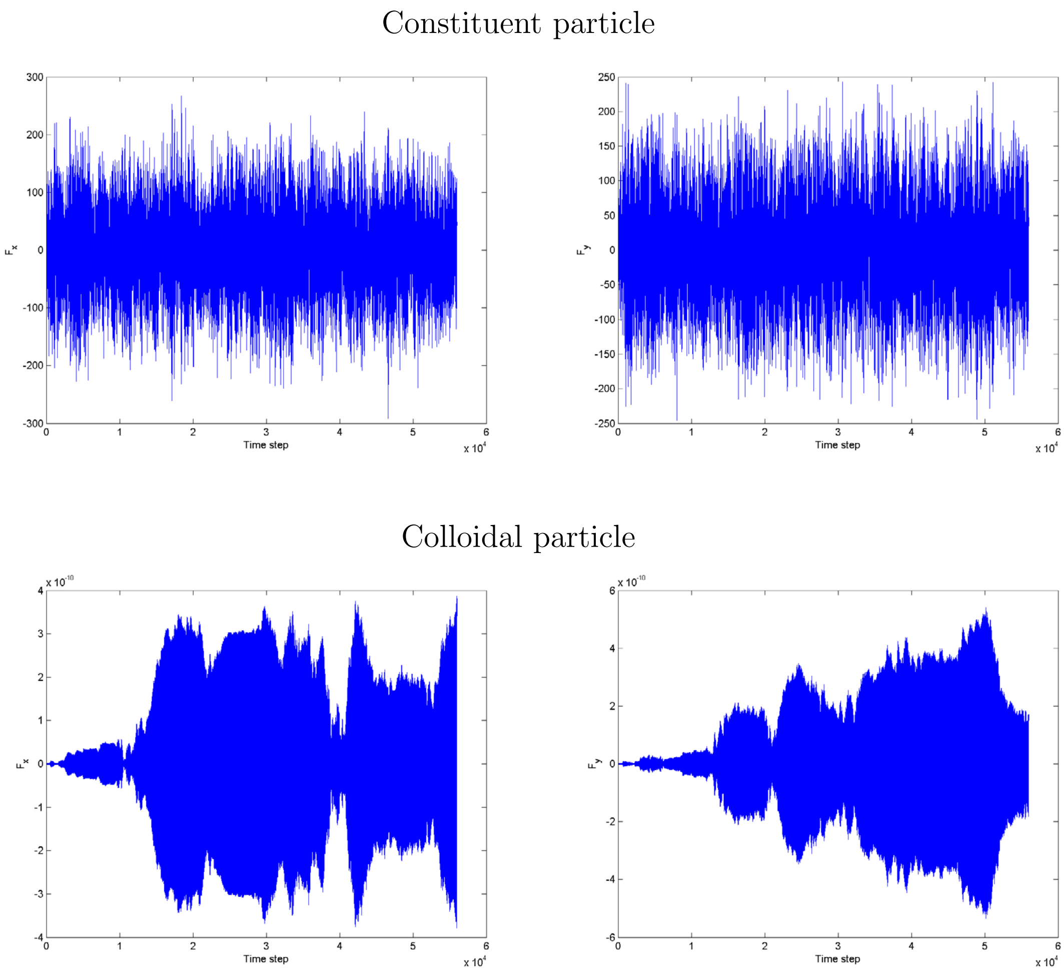

Figure 3: No flow, single colloidal particle, $\Delta t = 0.01$, $kBT = 1$: Spring forces on a constituent particle of the colloidal particle (top) and on the colloidal particle (bottom) in the x (left) and y (right) directions.

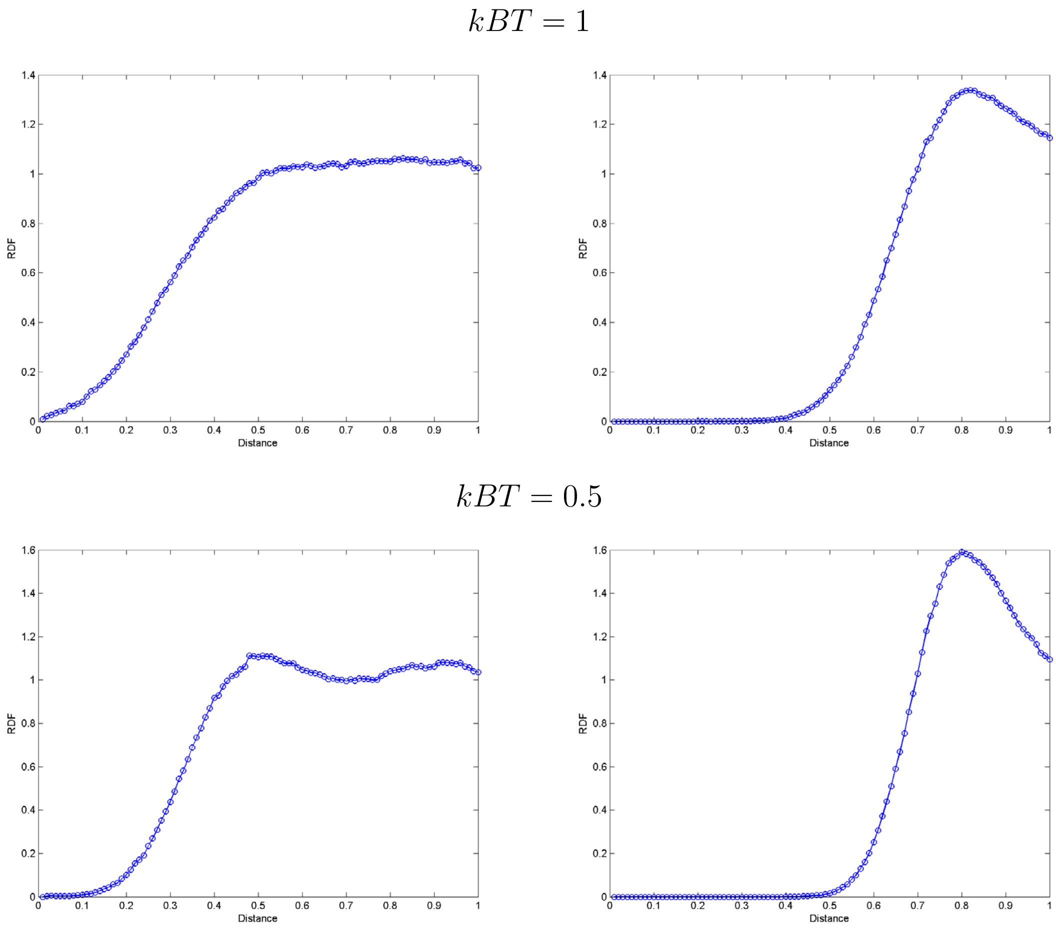

Figure 4: No flow, $\Delta t = 0.01$, 300000 time steps: radial distribution functions for the solvent (left) and colloidal (right) particles for two values of $k_B T$. All plots have the same length scale for the x axis.

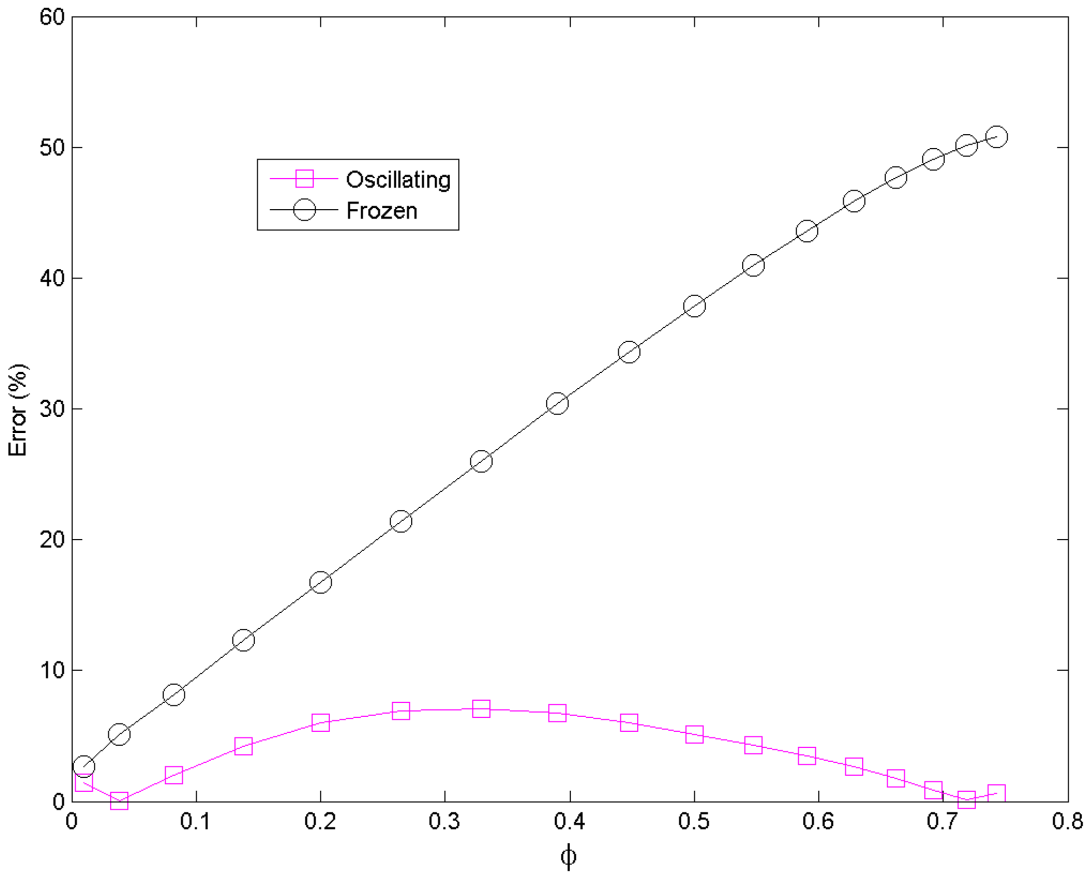

Figure 5: Shear flow, $\Delta t = 0.01$, $kBT = 1$, $U = 0.5$: Percentage error of average kBT over the entire domain versus volume fraction between the present oscillating and frozen particle models.

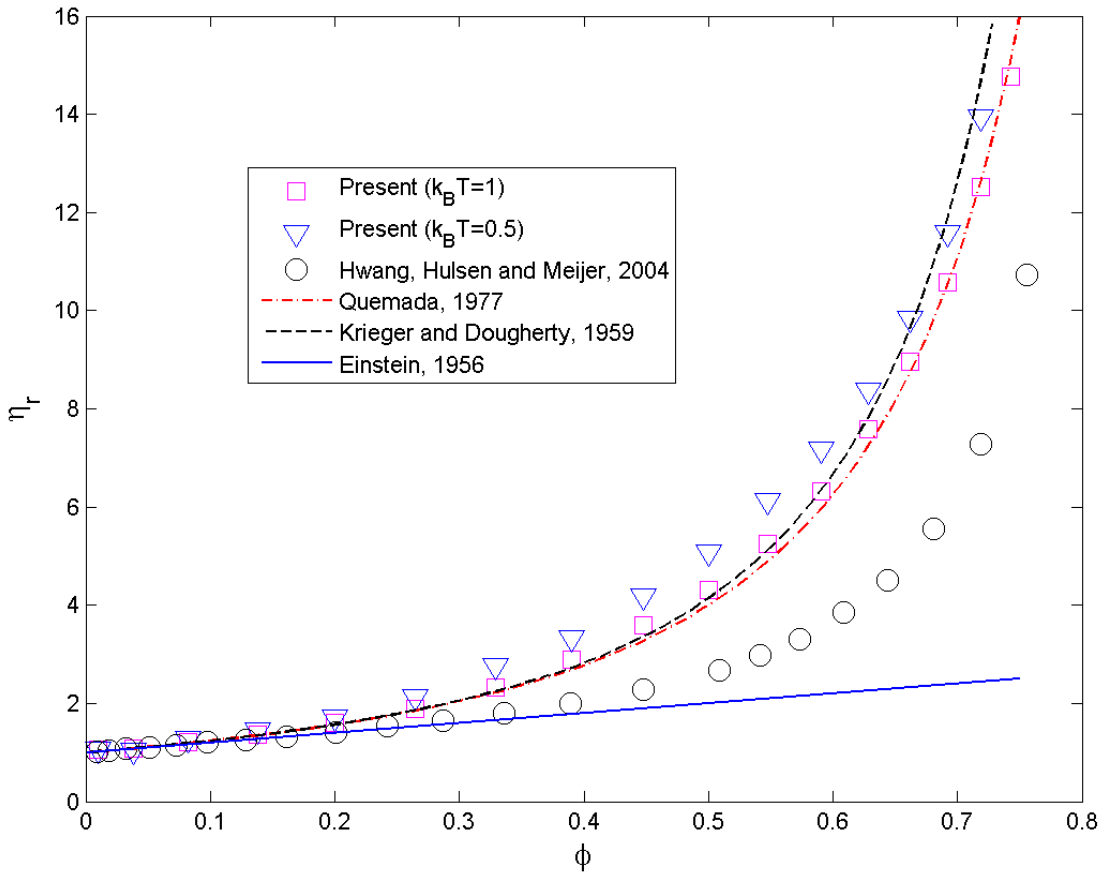

Figure 6: Shear flow, $\Delta t = 0.01$: zero-shear-rate relative viscosity versus volume fraction for $kBT = 1$ and $kBT = 0.5$.

REFERENCES

[1] Hoogerbrugge, P.J. and Koelman, J.M.V.A. Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics. *Europhysics Letters* (1992) **19(3)**:155-160.

[2] Español, P. Hydrodynamics from dissipative particle dynamics. *Phys. Rev. E* (1995) **52**:1734-1742.

[3] Español, P. and and Warren, P. Statistical mechanics of dissipative particle dynamics. *Europhysics Letters* (1995) **30(4)**:191-196.

[4] Koelman, J.M.V.A. and Hoogerbrugge, P.J. Dynamic simulations of hard-sphere suspensions under steady shear. *Europhysics Letters* (1993) **21(3)**:363-368.

[5] Pan, W., Caswell B. and Karniadakis, G.E. Rheology, microstructure and migration in Brownian colloidal suspensions. *Langmuir* (2010) **26(1)**:133-142.

[6] Hwang, W.R., Hulsen, M.A. and Meijer, H.E.H. Direct simulation of particle suspensions in sliding bi-periodic frames. *Journal of Computational Physics* (2004) **194(2)**:742-772.

[7] Quemada, D. Rheology of concentrated disperse systems and minimum energy dissipation principle. *Rheologica Acta* (1977) **16(1)**:82-94.

[8] Krieger, I.M. and Dougherty T.J. A mechanism for non-Newtonian flow in suspensions of rigid spheres. *Trans. Soc. Rheol.* (1959) **3**:137-152

[9] Einstein, A. *Investigations on the Theory of Brownian Movement*. Dover (1956).